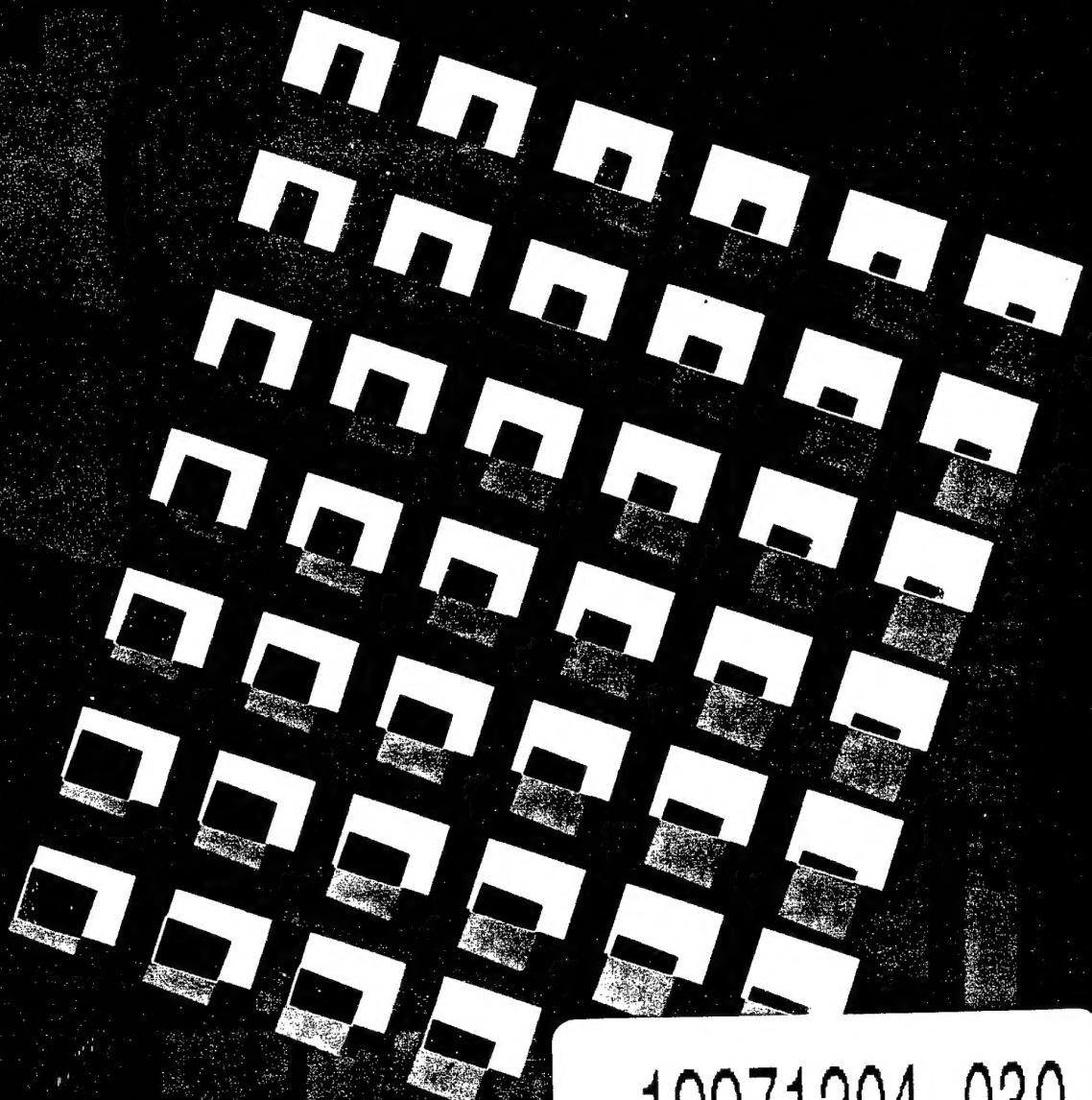
TNO report
PML 1997-A33

Shock Initiation Modelling of Explosives

TNO Prins Maurits Laboratory



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In dit rapport wordt een beschrijving gegeven van het modelleringswerk op het gebied van schokinitiatie van explosieve stoffen dat de laatste jaren is uitgevoerd op het TNO Prins Maurits Laboratorium (TNO-PML) in het kader van de opdracht A94KL482: Schokinitiatie Explosieve Stoffen. Het modelleringswerk heeft er zich enerzijds speciaal op gericht om de verschillen te beschrijven in het initiatiegedrag als gevolg van schokken van verschillende duur en vorm, corresponderend met de toegepaste experimentele initiatietechnieken, namelijk initiatie met een explosieve lading en initiatie door inslag met hoge snelheid van een dun kunststof folie. Anderzijds is speciaal gekeken naar de invloed van de grootte en grootteverdeling van de springstofdeeltjes op het initiatiegedrag.

Als basis van de modellering heeft gediend het Lee-Tarver model, een semi-empirisch initiatiemodel waarin het initiatieproces wordt gesplitst in twee fasen, een ontstekingsfase, waarin de creatie van zogenaamde 'hot spots' plaatsvindt, en een groeifase, waarin de verbranding van de springstofdeeltjes plaatsvindt. Gebruikmakend van dit model zijn simulaties uitgevoerd met behulp van de hydrocode Autodyn. Hierbij bleek dat hoewel een aantal schokinitiatieaspecten goed beschreven kunnen worden met het Lee-Tarver model, het met dit model toch niet mogelijk is om de experimenteel waargenomen verschillen in initiatiegedrag als gevolg van deeltjesgrootteverschillen te verklaren. Met name de beschrijving van de ontstekingsfase in het model bleek ontoereikend te zijn.

Om het schokinitiatiemodel aan te passen is voor de ontstekingsfase gebruikgemaakt van een zogenaamd viscoplastisch holte-implosie model. Hierbij wordt de creatie van hot spots ten gevolge van viscoplastische stroming bij de implosie van holtes in het materiaal beschreven. Van de verschillende in de literatuur beschreven modellen is het model van Khasainov et al. uitgekozen voor implementatie in Autodyn. Hiermee is een aantal simulaties uitgevoerd waarmee het inderdaad mogelijk bleek om sommige deeltjesgrootte-effecten kwalitatief goed te beschrijven.

Hoewel het model nog verder verbeterd zal moeten worden hebben de eerste resultaten met het aangepaste model aangetoond dat dit model een geschikte basis vormt om op voort te bouwen teneinde tot een beter begrip en een betere beschrijving te komen van de processen die plaatsvinden bij schokinitiatie.

Contents

1 Introduction

The purpose of assignment A94KL482: 'Schokinitiatie Explosieve Stoffen' is to keep available and further advance knowledge and skills on the subject of detonation properties and shock initiation of explosive materials. The knowledge and skills are essential to be able to advise the Royal Netherlands Military Forces in the future on the topics of purchase and use of ammunition systems.

Part of the assignment is to study the difference in initiation behaviour between initiation with a flyer plate and initiation with a booster charge. These two methods deliver a considerably different initiating shock pulse, where the differences are found in both length and height of the pulse and its shape. To study the initiation behaviour, a theoretical effort is needed besides the experimental work. In this respect, computer simulations are used to test various shock initiation models and to compare the results with the outcome of the experimental work.

In the past, several theoretical shock initiation models have been evaluated and incorporated into the computer code Autodyn that is in use at the TNO Prins Maurits Laboratory (TNO-PML). The starting point for this effort has been the Lee-Tarver shock initiation model, which is intrinsic to Autodyn. By applying some changes to this model, an attempt has been made to bring it further in line with the state of knowledge of the shock initiation process and with the experimental results, produced with the TNO Mega Ampere Pulser and the TNO gap test.

In the following sections, a description is given of the Lee-Tarver model and its implementation in Autodyn and of the adjustments applied to this model. An overview of the state of affairs in shock initiation modelling is given, and it is shown how the shock initiation model in Autodyn has been altered to reflect these models. Further, a short survey of the experimental results is given and the results are compared with the outcome of the various models. Finally, it is indicated how the model can be improved.

2 The Lee-Tarver shock initiation model

The Lee-Tarver or ignition and growth shock initiation model is basically a phenomenological model that has been developed at the Lawrence Livermore National Laboratory (LLNL) [1, 2]. It essentially consists of an equation for the reaction rate of the explosive as a function of a number of parameters. The model tries to give a generalized description of the underlying physical and chemical processes, making it possible to describe the shock initiation process irrespective of the geometry, the pulse-strength and -shape and other circumstances. However, it does not give a description of the microscopic phenomena that are taking place, such as nucleation, plastic flow and turbulent combustion, for example, but instead it divides the shock initiation process into a number of different stages and gives a simplified, phenomenological description of each stage. The rationale behind the division into stages is that in the past decades, experimental evidence has accumulated that the shock initiation process in heterogeneous explosives indeed breaks up into a number of clearly distinguishable stages; one being an ignition phase where so-called hot spots are created as a direct result of the impact of the leading shock wave and at least one growth stage where the build-up of chemical reaction takes place. The evidence has notably come from experiments with impacting thin flyer plates, using measurement techniques like manganin gauges, embedded particle velocity gauges, VISAR velocity measurements, fast framing cameras, etc.. It is generally believed that the ignition of the explosive occurs when the reaction grows outward from these reaction sites. The formation of hot spots can be explained by several plausible mechanisms, for example void closure, micro-jetting in collapsing voids, plastic work at void peripheries and friction between particles. The reaction growth occurring after the ignition stage is viewed largely similar to the deflagration process occurring in grain burning.

The Lee-Tarver model tries to give a description of the shock initiation process in agreement with the picture of the process, outlined above. In the original version of the model [1], two terms are used; the first describing the ignition stage and the second describing the growth stage. This results in the following equation:

$$\frac{dF}{dt} = I(1-F)^b \mu^x + G(1-F)^b F^g P^z \qquad (1)$$

where μ is the compression ($\mu = \rho / \rho_0 - 1$), F is the mass fraction of reacted explosive and I, b, x, G, g and z are constants.

The ignition term in the above equation is assumed to be proportional to some power of the compression. The value assigned to the exponent, x, depends on the hot spot formation model that is considered. Some models consider the ignition to be proportional to the square of the particle velocity u_p, while in others it is proportional to the square of the pressure P. Since to a good approximation P is proportional to μ^2 and u_p is proportional to $\mu^{3/2}$, in most simulations a value of 3 or 4

is assigned to x. The growth term in the above equation represents a pressure dependent laminar grain burning rate. Here the pressure exponent z usually lies between 1 and 2. The factor F^g is proportional to the burning surface area and, in the case of a spherical hot spot burning outward, the exponent has a value of 2/3. The proportionality constant G must be determined from laminar burn rate experiments. The factor $(1 - F)^b$ has been inserted to assure that the reaction rate equals zero when the fraction solid explosive approaches zero. The exponent b is given a value of 2/9 so that $(1 - F)^b$. F^g is at a maximum when F equals 3/4.

The parameters in equation 1 are determined in such a way that they give the best fit to the experimental data. In this process usually the parameters b and g are kept at constant values of 2/9 and 2/3, respectively, while x is given a value of either 4 or 3. The parameters z and G are varied in the fitting process but are not allowed to depart too much from known grain burning data. No restrictions apply to the parameter I.

With the above model, it appeared possible to describe successfully a great deal of experimental data on several explosives, including embedded pressure gauge and particle gauge data, VISAR data, gap test data and detonation failure data. However, when modelling short pulse duration shock initiation experiments, it appears to be necessary to increase the coefficient for the growth of reaction G by a factor of two or three, depending on the pressure. In order to be able to accurately model initiation caused by a wide variety of input pressures, rise times and pulse durations, the model has been adjusted [2] therefore, resulting in the following three-term reaction-rate equation:

$$\frac{dF}{dt} = I(1-F)^b(\mu - a)^x + G_1(1-F)^c F^d P^y + G_2(1-F)^e F^g P^z \qquad (2)$$

This equation contains 12 unknown parameters: I, b, a, x, G_1, c, d, y, G_2, e, g and z. In order to better limit the range of application of the three terms, three more constants have been added: F_{igmax}, F_{G1max} and F_{G2min}. The ignition in the reaction rate equation is set to zero when the fraction reacted material F exceeds F_{igmax} and, likewise, the first growth term is set to zero when F exceeds F_{G1max}. The second growth term is kept zero, while F is below the value F_{G2min}.

Compared to the first version of the model, the major difference is the growth term that has been split into two parts. The rationale behind this is that the relatively slow growth of reaction in deflagration-like grain burning only applies when the hot spots are still distinct. When the hot spots begin to coalesce, a fast decomposition of the remaining pockets of unreacted explosive will result and this can be modelled by a pressure-dependent growth rate with an exponent of 2 or 3. In the first growth term, a pressure exponent of 1 is used. Another change to this slow growth term is that the burning model has been changed from an outward hole burning model to an inward grain burning model, since this appeared to yield a better correlation with experimental data. The real geometry of reacting hot spots

is of course much more complex than either of the two burning models, and therefore it has been decided to choose the model that fits the experiments best. As a result, now the parameter c is taken to be 2/3, while the parameter d is set to 1/9. Except for the parameter z, the parameters in the fast growth term no longer have a clear relation to experimental burning rate data and are more or less used as fitting parameters, which is also true for the coefficient G_1 in the slow-growth term.

The form of the ignition term has hardly changed, but the values of the parameters used have been changed to account for experimental results. It appeared especially necessary to insure that for high input pressures and short pulse durations, a larger fraction of the explosive is ignited. This has been done by increasing the dependence of the amount of explosive ignited on the degree of the shock compression, thereby igniting much more explosive at high pressures approaching detonation pressures and much less explosive at low input pressures. Also, an extra parameter a has been added, providing a critical compression that is used to prohibit ignition until a certain degree of compression has been reached. Further, the value of the parameter b has been changed from 2/9 to 2/3 in accordance with parameter c.

In Table 1, as an example, the values of the reaction rate parameters are given for a number of explosives for both the 1980 and the 1985 model. Especially notable are the large differences in the ignition parameters I and x; both between the various explosives and between the two versions of the model. From these data and the explanation given above, it is clear that the emphasis in the 1985 model has shifted to a large extent to an approach where the parameters are determined by fitting the reaction rate equation to a large number of different experimental data. It has become much more difficult to give estimates of the parameters for newly developed energetic materials. This means that to obtain reasonably reliable parameter values for an explosive, many different experiments have to be carried out. As a consequence, reaction rate parameters are known only for a small number of explosives. For explosives for which not enough experimental data are available, it will therefore be difficult to reliably calculate shock initiation with a hydrocode using the Lee-Tarver model in an absolute sense. For such explosives, the best use of the model lies in the possibilities it offers for parameter variations. The relation between model parameters and explosive parameters is strong enough to be able to test variations in model parameters against variations in explosive properties.

Originally at LLNL, the Lee-Tarver model was incorporated into a special version of the one-dimensional Lagrangian Hydrocode KOVEC[3]. Later the model was implemented in the two- and three-dimensional versions of the Lagrangian finite element code DYNA [4]. In both implementations, in addition to the reaction rate equation, the JWL equation of state [5] has been used in the ignition and growth calculations for both the unreacted explosives and their reaction products.

Table 1: Lee-Tarver model parameters for some explosive materials [1, 2].

Material	PBX9404	TATB	PETN	Cast TNT	PBX9404	LX17	Propellant[1]
Model	1980	1980	1980	1980	1985	1985	1985
I (μs^{-1})	44	50	20	50	7.43×10^{11}	4.00×10^{6}	40
a	-	-	-	-	0.0	0.22	0.0
b	2/9	2/9	2/9	2/9	2/3	2/3	2/3
x	4	4	4	4	20	7	4
G_1 ($GPa^{-y}\mu s^{-1}$)	-	-	-	-	0.031	0.006	0.031
c	-	-	-	-	2/3	2/3	2/3
d	-	-	-	-	1/9	1/9	1/9
y	-	-	-	-	1	1	1
G_2,G ($GPa^{-z}\mu s^{-1}$)	0.126	0.0125	0.634	0.159	0.04	0.0004	0.0018
e	2/9	2/9	2/9	2/9	1/3	1/3	1
g	2/3	2/3	2/3	2/3	1	1	1/9
z	1.6	2.0	1.4	1.2	2	3	2
F_{igmax}	-	-	-	-	0.3	0.5	0.015
F_{G1max}	-	-	-	-	0.5	0.5	0.12
F_{G2min}	-	-	-	-	0.0	0.0	0.0

1 This propellant consists of AP, Al, HMX (12%) and a binder.

For unreacted explosives, the equation of state is fitted to the initial sound velocity and experimental Hugoniot data, and the initial internal energy is adjusted to make $P = 0$ when $\rho = \rho_0$ at the initial temperature. This unusual application of an equation of state, developed for the description of gases, to a solid material was preferred to the use of a linear shock equation of state. With the above construction, the JWL equation can both accommodate the measured bulk sound velocity and the experimentally observed curvature of the shock velocity-particle velocity relationship at higher shock pressures. In the calculation of the parameters of the mixture of solid and gases, it has been assumed that the pressures of both phases are in equilibrium and that their volumes are additive. It is however assumed that the temperatures of the reacted and unreacted material are not in equilibrium.

3 Implementation of the Lee-Tarver model in Autodyn

3.1 Autodyn

Autodyn is a hydrocode that is being used by several groups in TNO-PML for the simulation of various phenomena like penetration mechanics, blast modelling, explosive compaction of powders, propagation of shock waves and detonation waves, etc.. It is a commercial hydrocode, developed and marketed by the company Century Dynamics Inc. [6, 7]. It is related to the PISCES code (developed originally by Physics International) and as such it is a descendent of the HEMP code, developed at LLNL. It is available in a two-dimensional and a three-dimensional version. The code uses a finite difference technique and includes, among other things, both a Lagrange and an Euler processor. Being a commercial hydrocode, Autodyn is available only in binary form. It is therefore not possible to adjust the source code of the program for local purposes. Autodyn however supplies an interface by which user written subroutines, for example for the implementation of a new equation of state or material model, can be coupled to the code. This mechanism has been used for the implementation of the Lee-Tarver model in Autodyn, to be described below. Like the other codes, Autodyn is based on differential equations derived from the conservation laws of mass, momentum and energy. These are supplemented by a number of equations of state and material models, and when the boundary and initial conditions for the problem have been supplied, it is solved by an explicit time integration scheme. Among the many material models and equations of state available, there is also the JWL equation of state, which describes the behaviour of explosive materials.

3.2 Implementation of Lee-Tarver model

The implementation of the Lee-Tarver model in Autodyn was carried out by D. Davison of Shock Transients Inc. [8] under contract for Century Dynamics Inc.. The model was originally incorporated using the EXEOS user subroutine. Starting with version 3.0 of Autodyn, the model is a standard component of the available material models. The implementation differs from the LLNL implementation in that as equation of state for the solid material, instead of a JWL form, a shock equation of state is used, similar to the standard shock equation of state in Autodyn. This was chosen because the coefficients for the shock equation of state are more widely available. As input parameters for the calculation, apart from the reaction-rate parameters, the JWL parameters and the shock EOS parameters, the detonation velocity D, pressure P_{CJ} and internal energy E_{CJ} are also needed. Two extra input parameters, WREAC and DFMAX, determine the nominal reaction zone width and the maximum change in the ratio between reacted and unreacted

material in a time step. These latter two parameters can be used to control the stability of the calculation. The parameters D and P_{CJ} are only used as reference values in the calculations to control parameters such as the time step, and to provide extreme limits to the calculated pressure. Their values are not at all crucial to the outcome of the simulations and can be described adequately by rough estimates. Because of the conformity of the 1980 and 1985 versions of the model, both versions can be used in this implementation. To use the 1980 model, it is sufficient to set all parameters in the slow-growth term to zero and also make F_{G1max} equal to zero. The parameter values for the 1980 model can then be inserted in the parameters of the ignition term and the fast-growth term.

3.3 Shock initiation examples

In Figure 1, a typical example is given of a one-dimensional simulation carried out with the Lee-Tarver model in Autodyn. The situation modelled is that of a sustained shock pulse with a height of 6 GPa on a sample of an RDX-based Plastic Bonded Explosive (PBX). In the figure, a number of pressure profile plots is shown for different points of time. Initially, a steadily progressing shock wave is observed of which the amplitude is only slightly increasing. At a later stage, well behind the shock front, a pressure spike develops that quickly grows to a large amplitude and starts to gain on the shock front. After some time this pressure spike overtakes the shock front and a full detonation has developed.

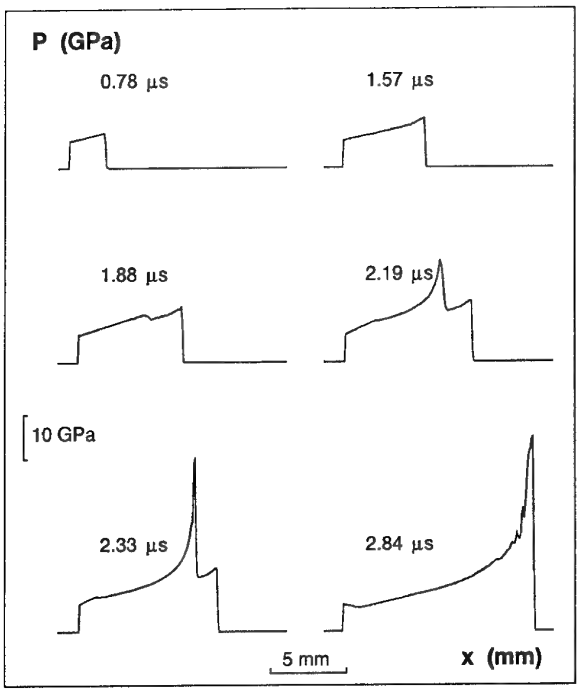

Figure 1: Development of pressure profiles in time for initiation with a 6 GPa shock.

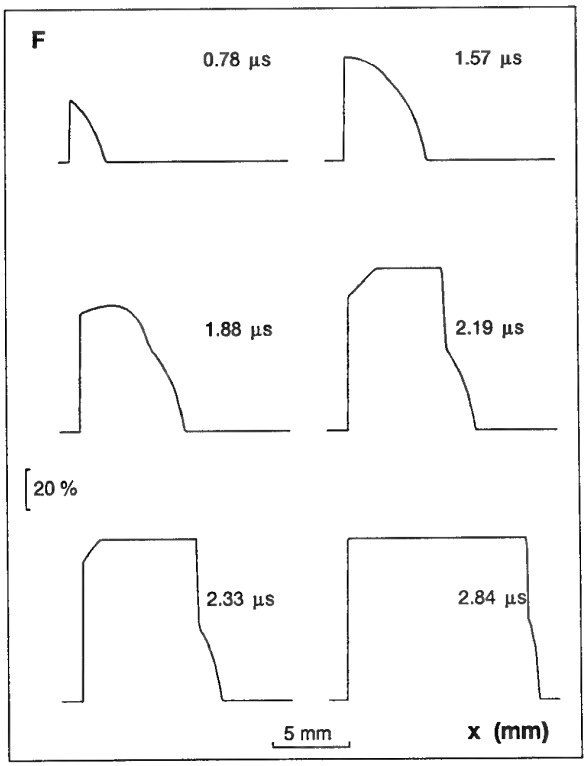

Figure 2: Reacted fraction profiles for the simulation of Figure 1.

The explanation for this behaviour can be found in Figure 2. In this figure, for the same points of time, the profiles ot the reacted fraction F are shown. The figure shows that at the shock front, only part of the material has reacted and that the growth of reaction continues behind the front, eventually accelerates and reaches completion well behind the front, giving rise to a local pressure spike. For shock pulses of low strength, this results in a very long reaction zone, the length of which is determined mainly by the length of the growth stage. Below a certain strength or for pulses with a too short duration, the reaction will not come to completion and the shock wave will eventually damp out.

4 Experimental shock initiation results

At TNO-PML, mainly two types of experiments are performed to measure the shock sensitivity of explosive materials. One is a gap test, where Hexocire (an RDX-wax mixture produced by SNPE, France) is used as donor explosive (diameter 50 mm, height 25 mm, density 1.54 mg/mm^3), and PMMA as gap material. With the use of a light source and an optical streak camera, the moment at which the shock wave enters the acceptor explosive is determined. When, after a certain time interval, a detonation develops in the explosive, the time and location of the break out of the detonation at the side of the sample is determined. In this way the initiation time and distance are recorded. See Figure 3 for a schematic drawing of the test.

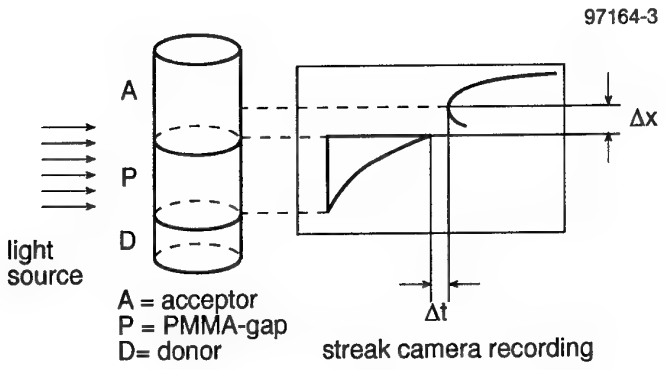

Figure 3: Schematic drawing of the gap test used at TNO-PML.

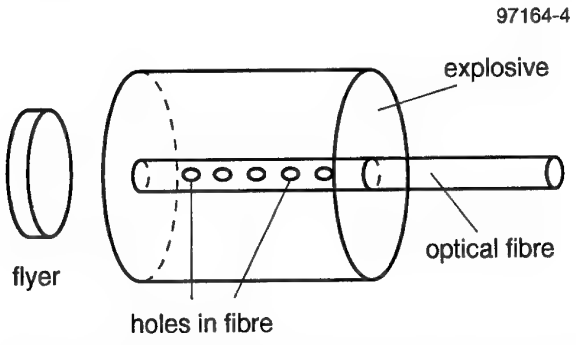

Figure 4: The thin flyer impact test with the Fibre Optic Probe.

The other type of initiation test that is in use at TNO-PML is a thin-flyer impact test, consisting of an electric gun and optical diagnostics. The electric gun is capable of launching kapton flyer plates with diameters of about 15 mm and a thickness of 125 µm or 250 µm to sufficiently high velocities to initiate most explosives. The optical diagnostics consist of 'time of flight' probes by which the shock front curvature can be determined and a 'fibre optic probe' by which the initiation time, the initiation distance and the detonation velocity in the explosive can be measured. See Figure 4 for a schematic drawing of the test.

With these two experimental set-ups, a number of HTPB-based PBX's (density=1.53 mg/mm^3) containing 65% of RDX have been tested. In these tests in particular, the dependence of the initiation behaviour on the particle size of the RDX particles has been studied. To this end, samples with four different crystal sizes have been prepared (see Table 2).

Table 2: Properties of the used RDX material in the preparation of HTPB-based PBX's.

	Particle diameter 50% (µm)	Particle diameter 10% - 90% (µm)	Specific Surface (10^3 mm^2/mm^3)
F1 (very fine)	4.7	2.2 - 10.7	1.65
F2 (fine)	47	27 - 73	0.1567
C1 (coarse)	234	177 - 315	0.0305
C2 (very coarse)	522	416 - 698	0.0124

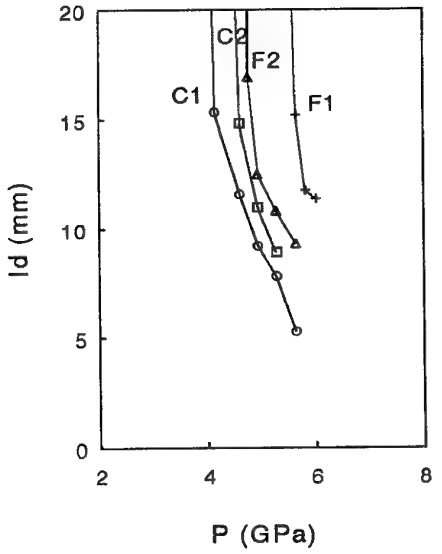

Figure 5: The initiation distance as a function of the input pressure measured with the TNO gap test for the RDX-PBX's for different grain sizes.

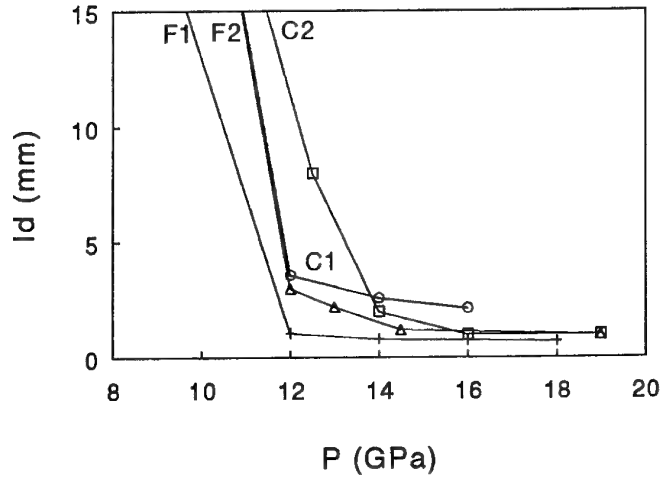

Figure 6: The initiation distance versus the input pressure for the 250 µm flyer impact experiments.

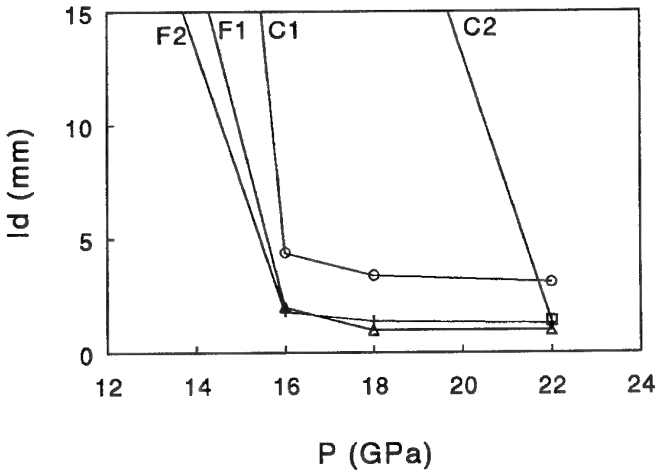

Figure 7: The initiation distance versus the input pressure for the 125 µm flyer impact experiments.

For these materials, both gap test experiments and flyer plate experiments with flyer thicknesses of 250 µm and 125 µm, respectively, providing shock pulses between 10 and 22 GPa and pulse durations between 40 and 100 ns were performed. In Figures 5 to 7, the results are given as plots of the initiation distance versus the impact pressure. From these figures it appears that the dependence of the sensitivity on the particle size is very different for long and short pulses. For the long pulses, generated with the gap test, the sensitivity decreases when the grain size becomes smaller. For the short pulses, generated by the flyer impact, on the other hand, the coarser particles appear to be less sensitive. Apart from the sensitivity, also the detonation velocity appears to depend on the particle size. For

an increasing grain size, the detonation velocity appears to decrease, even for sample diameters of 50 mm.

Comparable results have been obtained at Institute Saint Louis (ISL) by Moulard [9]. In their experiments also monomodal PBX's were tested with different RDX particle sizes. The PBX's consisted of 70% RDX and 30% polyurethane and had a density of 1.45 mg/mm^3. Three different RDX particle sizes were used, being respectively 6, 134 and 428 µm. The initiating shocks were generated by the impact of 8 mm thick aluminium-alloy flyer plates, having velocities between 1100 m/s and 2300 m/s, while the wedge test technique was used to monitor the response of the explosive material. The pulse durations generated were in the order of 2 µs and were longer than in the case of the TNO-PML thin-flyer experiments but shorter than in the case of the TNO-PML gap test. In these experiments, the coarse formulations appeared to be the most sensitive for low shock pressures, while for the higher shock pressures, the fine formulation was the most sensitive. The sensitivity curves appear to cross each other, as shown in Figure 8.

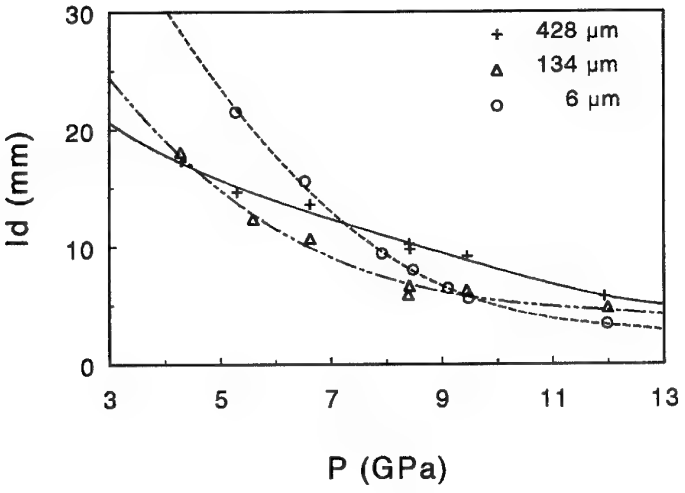

Figure 8: The initiation distance versus the input pressure for the ISL experiments.

From the above results, it becomes clear that both the shock duration and the particle size have a very important influence on the shock initiation behaviour. Therefore the simulation and modelling work have concentrated on trying to understand and model these influences.

5 Parameter variations with the Lee-Tarver model

With the Lee-Tarver model, discussed in sections 2 and 3, it is very difficult to quantitatively simulate the initiation experiments. In order to perform quantitative simulations, it is necessary to obtain adequate values for all 15 parameters of the used explosive composition. This requires a very large number of experiments for each explosive formulation. Therefore the main use of the simulations at TNO-PML is as a tool to qualitatively examine the influence on shock initiation behaviour of changes in parameters of the explosive material.

Table 3: Lee-Tarver model parameters used in the simulations.

Parameter	Value
I (μs^{-1})	10^{-3} - 10^{4}
a	0
b	0.1
x	4
G_1 ($GPa^{-y}\mu s^{-1}$)	0.05 - 0.3
c	0.667
d	0.083
y	1
G_2 ($GPa^{-z}\mu s^{-1}$)	2.25 x 10^{-3}
e	0.222
g	0.667
z	3
F_{igmax}	0.3
F_{G1max}	0.5
F_{G2min}	0.5

A number of parameter variations have been carried out to examine the relative influence on the shock initiation process of the different terms in the initiation model. To this end, especially the proportionality constants I and G_1 of respectively the ignition term and the first growth term have been varied. The values of the parameters used are given in Table 3. These values are representative for the kind of RDX-based PBX's used in the experiments, but they do not provide a precise description of the initiation behaviour of the actual PBX's. Several series of simulations were performed for a number of I, G_1 combinations. While the parameter I was fixed to a value of 10 μs^{-1}, simulations were carried out with G_1 varying between 0.05 $GPa^{-1}\mu s^{-1}$ and 0.3 $GPa^{-1}\mu s^{-1}$, and with G_1 fixed to 0.01 $GPa^{-1}\mu s^{-1}$, the parameter I was varied between $10^{-3}\mu s^{-1}$ and $10^{4}\mu s^{-1}$. These simulations were performed in a one-dimensional geometry for sustained shock pulses with pulse heights between 4 and 10 GPa.

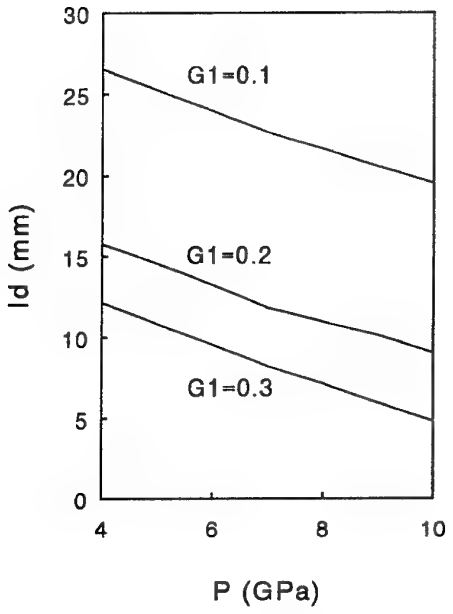

Figure 9: Initiation distance as a function of pressure for various values of G_1.

In Figure 9, a plot is given of the initiation distance as a function of the initiation pressure for various values of the amplitude G_1 of the growth term. In this plot and in the following plots, no clear pressure threshold for shock initiation can be observed. This is due to limitations in the Lee-Tarver model and to the fact that the simulations have been carried out in one dimension. Two-dimensional simulations, not shown here, do show an initiation threshold. In the plots, the sensitivity to shock initiation is judged from the initiation distance. Figure 9 shows the influence of G_1 on the initiation distance, while all other parameters are kept constant. This influence appears to be rather strong. On the other hand, the influence of varying the amplitude I of the ignition term, shown in Figure 10, appears to be rather limited. 'I' had to be increased by a factor of 10000 to reduce the initiation distance by no more than 25%. Increasing 'I' still further did not result in a shorter initiation distance. An important reason for this phenomenon is that in the model, the ignition term is only active till a reacted fraction F_{igmax} is reached. Above that limit only the growth terms contribute to the reaction rate. It appears that the growth terms to a great extent determine the value of the run distance to detonation. On the other hand, the ignition term determines whether the explosive is sufficiently ignited to start an accelerating reaction.

Similar simulations have also been performed for shock pulses with a shock duration between 100 ns and 1 µs. For pulses shorter than 600 ns, the initiation distance starts to increase. However, also for these short pulses the influence of parameter variations of I and G_1 stays essentially the same, although the relative influence of I compared to G_1 is much larger than for sustained pulses. In Figure 11 the influence is shown of the pulse length on the initiation distance for several shock pressures. Above a certain pressure-dependent pulse duration, the

initiation distance is independent of the pulse duration; while for short shocks, the initiation distance is a strong function of the shock length.

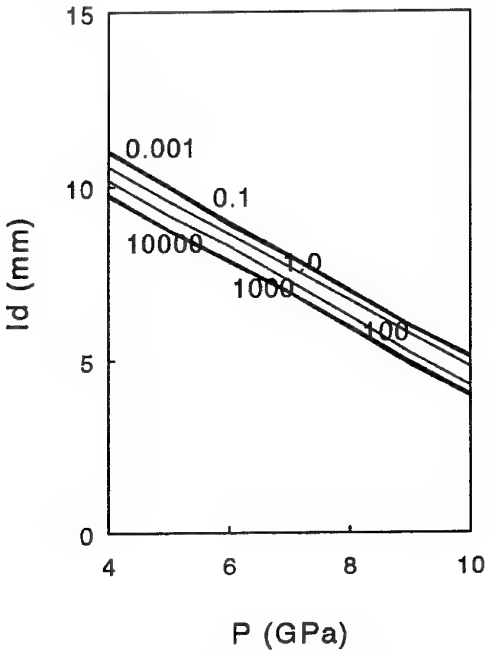

Figure 10: Initiation distance as a function of pressure for various values of I.

The simulations indicate that the growth terms have a much larger influence on the initiation distance than the ignition term. Although a direct correspondence between the properties of the explosive and the parameters of the model does not exist, for some properties, a clear relation exists with one of the terms in the model. In this respect we can expect that, for example, the particle size has a large influence on the growth terms because of the much larger burning surface that is provided by small grains. We would therefore expect that the parameter G_1 will be larger for smaller sizes. The influence of the particle size on the ignition term is more difficult to estimate and will be different for the different mechanisms that may be responsible for ignition like void closure, microjetting, plastic work at void peripheries, particle friction, etc.. Possibly these mechanisms are less likely to occur for small particle sizes. The particle shape and smoothness will probably have little influence on the parameters of the growth terms but will certainly affect the ignition process, although it is not clear how to correlate them with the parameters of the ignition term. From the outcome of the simulations, one may therefore conclude that the main effect of decreasing the particle diameter will be an increase of the value of G_1, resulting in a shorter run distance to detonation.

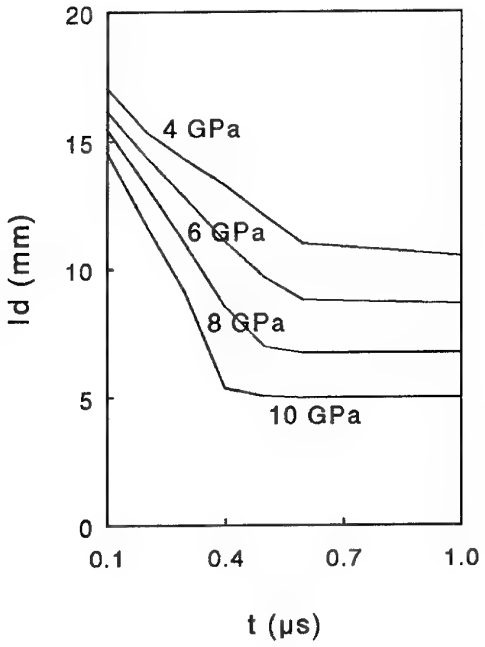

Figure 11: Influence of pulse duration on initiation distance for various shock pressures.

The prediction by the model of the dependency of the sensitivity on the particle size, as judged from the initiation distance, is not in agreement with the experimental results. For long pulses, even the opposite tendency can be observed.

The reason for the observed discrepancy can be twofold. In the first place the description of the ignition stage in the model is apparently insufficient. The model does not predict the sharp increase in initiation distance near the threshold, as observed experimentally, while the influence of the ignition stage on the total process is too small. On the other hand, experimental parameters that are not modelled in the simulations may play an important role. For example, two-dimensional effects such as the influence of rarefaction waves penetrating into the explosive from its sides may be important, while the influence of the binder material on the process is not known. Another complicating factor is the dependency of the detonation velocity on the particle size.

From the above it is clear that it is necessary to improve on the Lee-Tarver model in order to give a better description of especially the ignition process and to make it possible to better link the model parameters with the experimental parameters.

6 Viscoplastic pore-collapse initiation modelling

In order to give a better description of the experimental results, it is necessary to incorporate into the model a description of the ignition process that is less phenomenological and is closer to the mechanisms that are taking place during ignition. Processes that are considered important for initiation are particle friction, the collapse of pores in the material, plastic work performed at the peripheries of the pore and microjetting. Most modelling work that has been carried out recently in this respect has concentrated on describing hot spot creation due to the collapse of pores in the material. The heating of the material in such a process can be due to various mechanisms. In the initiation model of Mader [10], a hydrodynamic mechanism is considered, where the heating is produced by compression of the solid material. In the work of Bowden and Yoffe [11], the role of gas compression in the pores is emphasized. Carroll and Holt [12] consider heating due to inviscid, plastic flow during pore collapse, while Khasainov et al. [13], consider purely viscous plastic work. In all cases significant temperature rises are predicted for a thin shell of material around the collapsing cavity. An analysis by Frey [14] shows that of the above mechanisms, the viscoplastic work during pore collapse gives, in most cases, by far the most important contribution to the heating of the materials. Therefore, currently most shock initiation models are based on the viscoplastic pore collapse mechanism.

In the model of Khasainov et al. [13], the viscoplastic collapse of a hollow sphere with an inner radius a and an outer radius b is modelled. The inner radius a is equal to the average pore radius and the outer radius b is equal to the average distance between two voids. The porous material is then described as a suspension of pores inside a homogeneous, isotropic, ductile crystal matrix. This is of course a strong simplification of the actual geometry of the explosive material, but since the viscous collapse time is much longer than the time needed for a shock wave to cross the pore, it is not an unreasonable simplification. As in the pore collapse model of Carroll and Holt [12], it is assumed that the pore volume remains essentially unchanged until the pressure reaches the yield value P_y:

$$P_y = \frac{2}{3} Y \ln\left(\frac{b^3}{a^3}\right), \tag{3}$$

where Y is the plastic yield strength. In the model, the dynamic collapse of the cavity for pressures above P_y is calculated and the corresponding temperature rise in the vicinity of the pore. An ignition delay τ_{ig} can then be derived, using an Arrhenius type of reaction:

$$\tau_{ig} \approx \frac{4}{3} \frac{\rho_s c_s \mu_s \left(T_{ig} - T_0\right)}{\left(P_s - P_y\right)^2}, \tag{4}$$

where ρ_s, c_s and P_s are respectively the density, specific heat and pressure of the solid material, μ_s is the coefficient of viscosity, T_{ig} is the ignition temperature and T_0 is the starting temperature. After ignition, the reaction rate is described by a simple term $dF/dt = b\ P^x$, where b and x are constants.

The model of Belmas et al. [15] is similar to that of Khasainov. One of the differences is that in the former model, the cooling of the material due to thermal conduction is also incorporated. The model of Butler et al. [16] is more complex than the other pore collapse models, since a full description of the gas phase and the interaction between gas and solid phase has also been given. Further, chemical decomposition at the pore interface is considered, while also the role of gas phase chemistry has been investigated.

From the modelling work above, it is clear that the dependence of the reaction rate on the pore size during the ignition phase is different from the dependence during the growth phase, which makes the viscoplastic pore collapse mechanism a good candidate for explaining the experimental results, described in section 4. Therefore it was decided to incorporate such a model in Autodyn.

7 Implementation of pore-collapse model in Autodyn

The models, discussed in the previous section, cannot be incorporated directly into Autodyn. The models typically consist of a set of differential equations that are solved either analytically or numerically. For easy implementation into Autodyn, one needs something in the form of a burning rate law. Therefore we decided to make some changes to the implementation of the Lee-Tarver model, which is already implemented in Autodyn, more or less in agreement with the pore-collapse models described. For the ignition term, use is made of the formula for the ignition delay, given by Khasainov et al. (equation 4). This ignition delay is now interpreted as the time interval needed to create a small hot spot of reacted material. The average reaction rate $(dF/dt)_{ig}$ is then defined as:

$$\left(\frac{dF}{dt}\right)_{ig} = \frac{F_{igmax}}{\tau_{ig}}, \tag{5}$$

where F_{igmax} is the reacted fraction at the end of the ignition stage. This is only a small fraction, in the order of a few per cent. To take into account that the actual explosive materials do not actually consist of hollow spheres, we further introduce the parameter N, which is the number of pores per grain, with:

$$b = \frac{r_0}{N}, \tag{6}$$

where r_0 is the particle radius. From equations 3 to 6, one obtains the following expression for the ignition term:

$$\left(\frac{dF}{dt}\right)_{ig} = \tfrac{3}{4}\frac{1}{\rho_s c_s \mu_s \left(T_{ig} - T_0\right)}\left[P_s - \tfrac{2}{3} ln\left(\frac{r_0^{\,3}}{a^3 N^3}\right)\right]^2 F_{igmax} \tag{7}$$

With respect to the growth stage, only a small modification is applied to the first growth term in the adapted Lee-Tarver model:

$$\left(\frac{dF}{dt}\right)_{g1} = \frac{G_1}{r_0}(1-F)^c F^d P^y \tag{8}$$

The only difference is that a factor r_0 has been split off from the parameter G_1 to make G_1 more or less independent of the particle size r_0. The second growth term remains unchanged:

$$\left(\frac{dF}{dt}\right)_{g2} = G_2(1-F)^e F^g P^z \tag{9}$$

Another slight modification to the Lee-Tarver model is that the three terms are now never active together:

$$\left(\frac{dF}{dt}\right)_{ig} = 0 \qquad for\ F > F_{igmax} \tag{10}$$

$$\left(\frac{dF}{dt}\right)_{g1} = 0 \qquad for\ F < F_{igmax}\ and\ F > F_{G1max} \tag{11}$$

$$\left(\frac{dF}{dt}\right)_{g2} = 0 \qquad for\ F < F_{G2min} = F_{G1max} \tag{12}$$

Equations 7 to 12 represent the pore collapse model as implemented in Autodyn.

8 Results of simulations

Table 4: Geometrical model parameters used in the calculations.

	Grain radius r_0 (μm)	pore radius a (μm)	N
Fine grains	6.0	1.0	1
Coarse grains	50.0	4.0	8

With the model from section 7, a number of one-dimensional simulations have been carried out to test whether this model shows a better agreement with experimental results than the Lee-Tarver model. In the simulations, a rectangular shock pulse is applied to the grid with a pulse height varying between 0.2 GPa and 12 GPa and a pulse duration of 200 ns. In the simulations, two different grain sizes have been used, 6 μm and 50 μm (see Table 4). In Table 4, estimated values for the pore radius a and the number of pores per grain N are also given. The values of the other parameters used are given in Table 5.

Table 5: Other model parameters used in the calculations.

Parameter	Value
Y(GPa)	0.2
ρ_s (kg m^{-3})	1770.0
c_s (J kg^{-1} K^{-1})	1250.0
μ_s (Pa s)	50.0
$(T_{ig} - T_0)$ (K)	700.0
G_1 (GPa^{-y} μs^{-1} mm)	0.03
y	1.0
c	0.667
d	0.083
G_2 (GPa^{-z} μs^{-1})	0.03
e	0.222
g	0.667
z	3.0
F_{igmax}	0.05
F_{G1max}	0.4

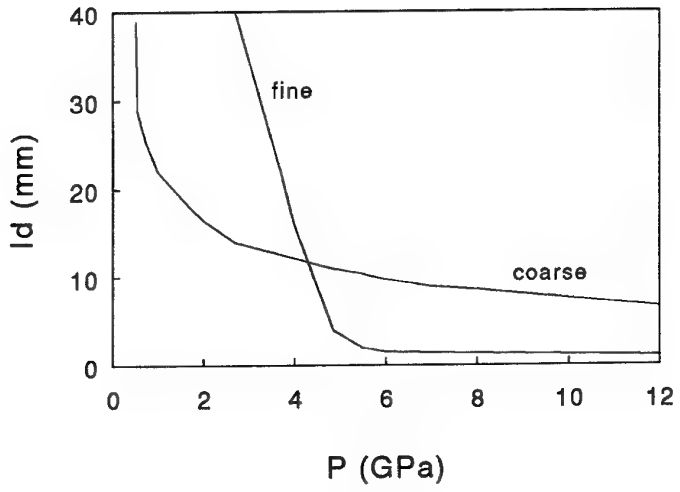

Figure 12: Initiation distance versus pressure for two different grain sizes.

In Figure 12, the results for these two particle sizes are given as a plot of the initiation distance versus the initiation pressure. From the figure it appears that for low shock pressures, the fine grains have a longer initiation distance; while for higher pressures the coarse grains have a longer initiation distance. Although these results cannot be compared directly with the experimental results of TNO-PML described in section 4, they do not contradict them. Further, they agree with the experimental results of Moulard [9], also described in section 4. The viscous porecollapse model therefore appears to have the potential to describe the dependencies of shock initiation on particle size that are experimentally observed.

9 Discussion

The adjustment of the Lee-Tarver model, described in section 5, has shown some promising results. It has been demonstrated that the revised model has the potential to correctly account for the particle size dependence of shock initiation. The approach is a provisional one and has to be improved further. Especially a better expression for the reaction rate during the ignition stage is desired. It also has to be examined whether a more sophisticated method is needed to describe the complex geometry than the currently used collection of hollow spheres.

Furthermore, it has to be pointed out that shock initiation due to implosion of empty cavities usually only occurs in pressed explosives. Cast explosives such as the PBX's mentioned in section 4 generally have a very low porosity and provide insufficient hot spots to initiate a detonation. However, these PBX's can be viewed as consisting of relatively large cavities, filled with binder and surrounded by explosive. These 'cavities' will partly collapse when hit by a shock wave due to the generally greater compressibility of the binder material with respect to the explosive. In this way the same model can be used to describe these explosives. The model should however be modified to include the compressibility of the binder. When doing so, the analysis that has been done by Frey [14] for empty cavities has to be repeated for this case in order to verify whether the viscoplastic pore-collapse mechanism is still the most important initiation mechanism. If it appears that other mechanisms become of comparable importance, it must be examined whether there is an easy way to incorporate also these mechanisms into the model.

The model in its current form still has to be tested further; especially its functioning in a two-dimensional geometry has to be examined. Then its behaviour at the occurrence of rarefaction waves and reflected shock waves can be tested and a better comparison with real experiments can be made. For instances, it can be examined whether the observed particle size dependence of the detonation velocity is explained by the model.

Although the model still needs to be improved, the first results with this provisional model have demonstrated that it has a large potential to explain a number of experimentally observed phenomena. By proceeding on this basis we can expect to reach a better understanding and to give a better description of the processes occurring at shock initiation.

10 Conclusion

In order to better understand and describe the experimental shock initiation results, obtained with RDX-based PBX's, a shock initiation model based on the viscoplastic core collapse initiation mechanism has been incorporated into the hydrocode Autodyn. The results obtained with the model in its current state show that some experimental results can already be explained. However, the model still needs further testing and will have to be further improved.

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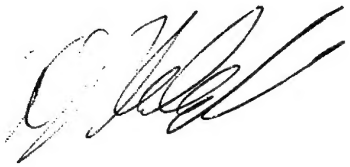
12 Authentication



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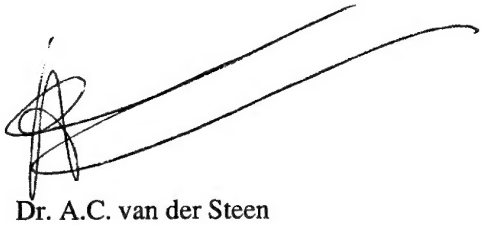

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15. ABSTRACT (MAXIMUM 200 WORDS (1044 BYTE))

In this report, a description is given of the modelling work on the subject of shock initiation of explosive materials that has been carried out at TNO Prins Maurits Laboratory (TNO-PML) in recent years. Initially, simulations were carried out with the Lee-Tarver shock initiation model, implemented in the hydrocode Autodyn. Although several aspects of shock initiation can be described satisfactorily with this model, the model cannot describe the experimentally observed dependencies of the initiation behaviour on the explosive particle size. Therefore the model has been adjusted by incorporating a viscoplastic pore collapse initiation mechanism, based on the work of Khasainov et al.. The first results obtained with the adjusted model show that some experimental results can already be explained and that the incorporation of the pore collapse mechanism is a good starting point for further development of the shock initiation model.

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